Machine Learning 1

Lecture 10.1 - Unsupervised Learning
Principal Component Analysis - Variance Maximization

Erik Bekkers

(Bishop 12.1.1)

Slide credits: Thomas Kipf, Giorgio Patrini

Image credit: Kirillm | Getty Images

Continuous latent space

Goal

- Dimensionality reduction: model the data in a low dim. space

- Example: take one grey-scale image of “3” and make multiple copies by translation and rotation

Figure: Synthetic “3” dataset (Bishop 12.1)

- Pixel space dimension: 100x100 pixels

- Latent space dimension: 3 = 2 (translations) + 1 rotation

- From the 3 latent variables we could generate all 100x100 pixels!

Example continued

- A more realistic dataset of images will have more degrees of freedom in the latent space, such as:
    - Scaling
    - Digits from 0-9
    - Colors
    - Different hand-writing styles
    - Etc.

  … but still much fewer than 100x100!

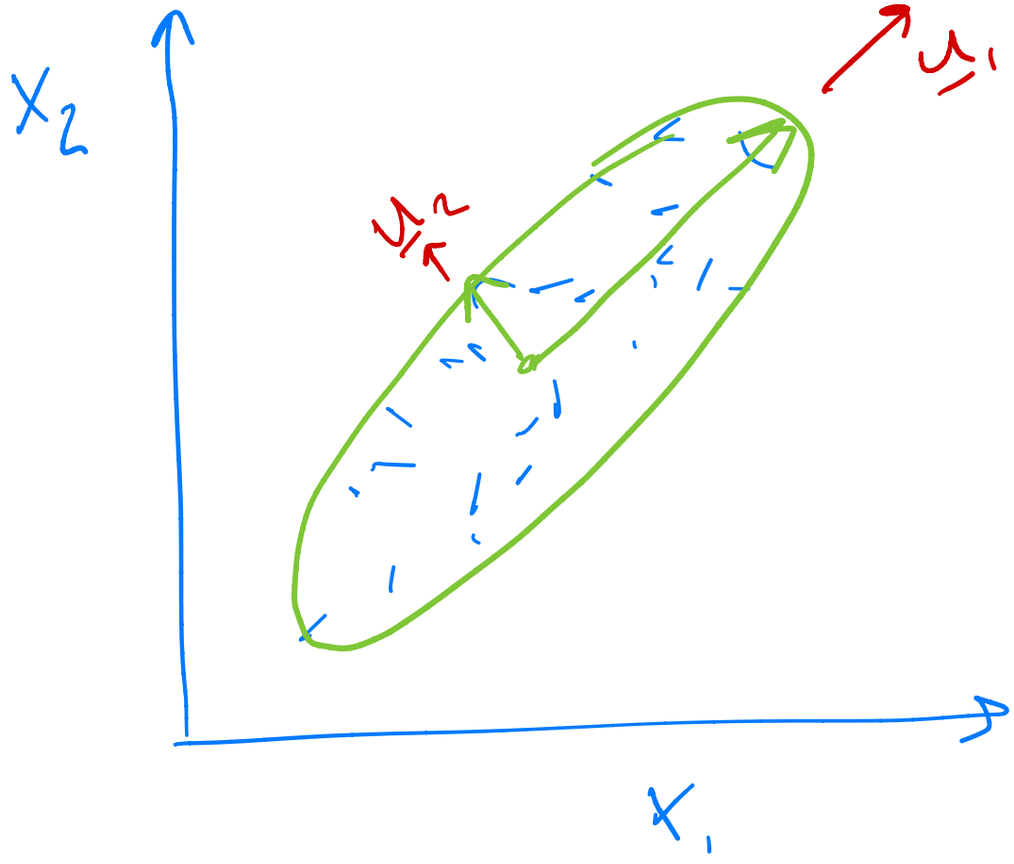
- In this example, the latent subspace is a non-linear transformation of the images

- We first study linear latent spaces with PCA and later consider generalizations to the non-linear case

Principal Component Analysis (PCA)

- Find a linear projection of the data such that the variance in the projected space is maximal

- PCA captures the axes of maximal variation in the data, called **principal components**



Principal Component Analysis (PCA)

- Data: $\mathbf{X} = \{\mathbf{x}_1, \ldots, \mathbf{x}_n\}, \;\; \mathbf{x}_n \in \mathbb{R}^D$

- Goal: project data into a $M < D$ dimensional space while **maximizing the variance** of the projected data

- M is given

- Mean and covariance defined by

$$\overline{\mathbf{x}} = \frac{1}{N} \sum_{n=1}^{N} \mathbf{x}_n$$

$$\mathbf{S} = \frac{1}{N} \sum_{n=1}^{N} (\mathbf{x}_n - \overline{\mathbf{x}})(\mathbf{x}_n - \overline{\mathbf{x}})^T$$

- $\mathbf{S}$ is symmetric and positive definite

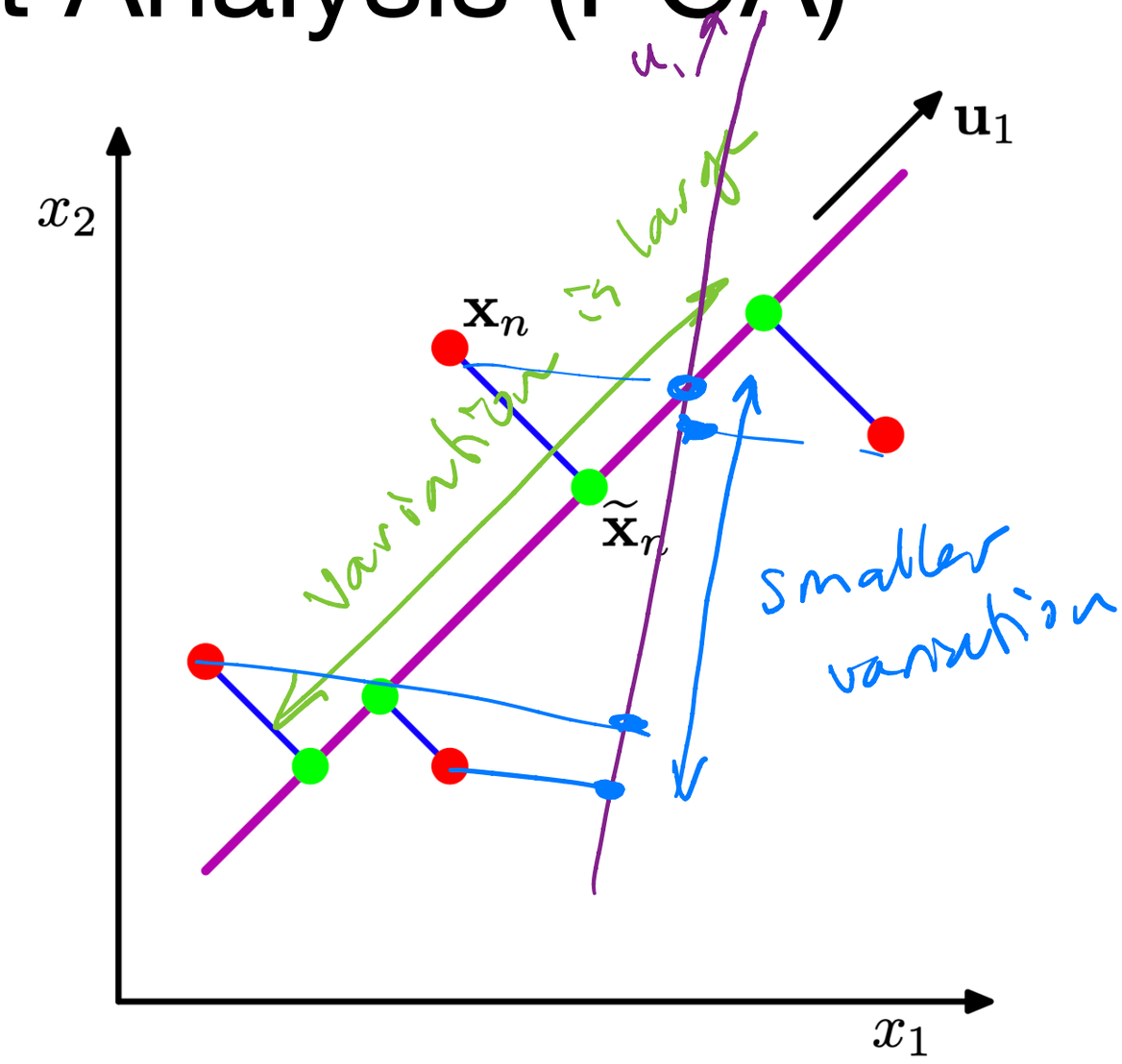


Figure: Maximizing variance of projections (Bishop 12.2)

1D Projection

- Project data int the first latent dimension by a vector $\mathbf{u}_1 \in \mathbb{R}^D$
- The projection gives the scalar $\mathbf{u}_1^T \mathbf{x}_n$, the mean of the projection is $\mathbf{u}_1^T \overline{\mathbf{x}}$
- We only need its direction, so normalize this component: $\|\mathbf{u}_1\|^2 = \mathbf{u}_1^T \mathbf{u}_1 = 1$
- The variance of the projected data is

$$\frac{1}{N} \sum_{n=1}^{N} (\mathbf{u}_1^T \mathbf{x}_n - \mathbf{u}_1^T \overline{\mathbf{x}})^2 = \frac{1}{N} \sum_{n=1}^{N} (\mathbf{u}_1^T (\mathbf{x}_n - \overline{\mathbf{x}}))^2$$

$$= \frac{1}{N} \sum_{n=1}^{N} \mathbf{u}_1^T (\mathbf{x}_n - \overline{\mathbf{x}})(\mathbf{x}_n - \overline{\mathbf{x}})^T \mathbf{u}_1$$

$$= \mathbf{u}_1^T \left(\frac{1}{N} \sum_{n=1}^{N} (\mathbf{x}_n - \overline{\mathbf{x}})(\mathbf{x}_n - \overline{\mathbf{x}})^T \right) \mathbf{u}_1 = \mathbf{u}_1^T \mathbf{S} \mathbf{u}_1$$

Maximizing the variance of 1 component

- Solve $\underset{\mathbf{u}_1}{\operatorname{argmax}}\ \mathbf{u}_1^T \mathbf{S}\, \mathbf{u}_1$ subject to $\mathbf{u}_1^T \mathbf{u}_1 = 1$

Need this constraint else objective is infinite

$\mathbf{u}_1^T \mathbf{S}\, \mathbf{u}_1 = f(\mathbf{u}_1)$, $\mathbf{u}_1^T \mathbf{u}_1 = g(\mathbf{u}_1) = c$

- Method of Lagrange multipliers
  - Define Lagrangian $L(\mathbf{u}_1, \lambda_1) = \mathbf{u}_1^T \mathbf{S}\, \mathbf{u}_1 + \lambda_1(\mathbf{u}_1^T \mathbf{u}_1 - 1)$

$f(\mathbf{u}_1)$ $\lambda_1(g(\mathbf{u}_1) - c)$

  - Solving for $\mathbf{u}_1$ means $\dfrac{\partial}{\partial \mathbf{u}_1} L(\mathbf{u}_1, \lambda_1) = \mathbf{S}\, \mathbf{u}_1 - \lambda_1 \mathbf{u}_1 = 0$
  - We need to solve eigensystem $\mathbf{S}\, \mathbf{u}_1 = \lambda_1 \mathbf{u}_1$
  - So $\mathbf{u}_1$ and λ_1 are respectively an eigenvector and eigenvalue of $\mathbf{S} \in \mathbb{R}^{D \times D}$!

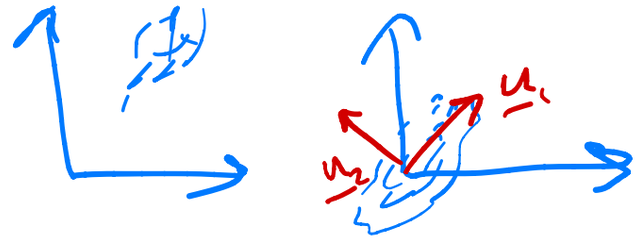
- The $\mathbf{u}_1$ is called a **principal component**.

$\mathbf{u}_1^T \lambda_1 \mathbf{u}_1 = \lambda_1 \mathbf{u}_1^T \mathbf{u}_1 = \lambda_1$

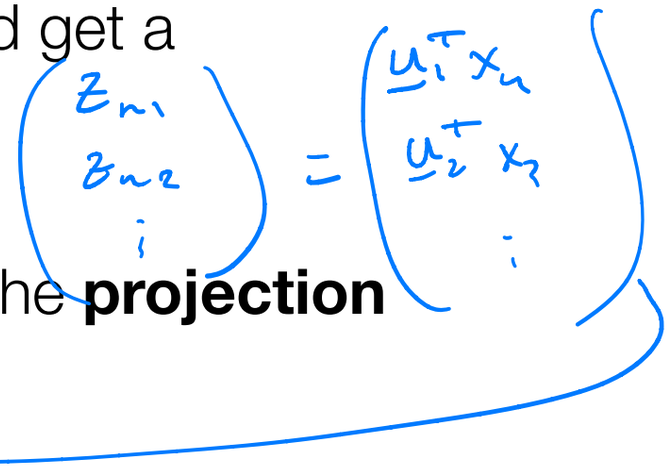
- The variance of the projected data is $\mathbf{u}_1^T \mathbf{S}\, \mathbf{u}_1 = \lambda_1$

- Maximizing variance means we search for the eigenvecor with **largest eigenvalue**

PCA via maximum variance



- We repeat the procedure for M orthogonal vectors and get a projection defined by $U_M = [\mathbf{u}_1, \ldots, \mathbf{u}_M] \in \mathbf{R}^{D \times M}$



- PCA: compute $\overline{\mathbf{x}}$ and the eigen-decomposition of $\mathbf{S}$. The **projection** then is $\mathbf{z} = \mathbf{U}_M^T(\mathbf{x} - \overline{\mathbf{x}})$

- Those are M eigenvectors of $\mathbf{S}$, **the principal components**. The eigenvalues are $\lambda_1 \geq \lambda_2 \geq \ldots \geq \lambda_M$

- The matrix $\mathbf{S}$ is positive semi-definite, thus $\forall_j : \lambda_j \geq 0$

- The (total) variance of the projected data is $\mathbf{Tr}[\mathbf{Cov}[\mathbf{z}]] = \sum_{j=1}^{M} \lambda_j$

Reminder: eigen-decomposition

$\underline{u}_i^T \underline{u}_j = \begin{cases} 1 & \text{if } i = j \\ 0 & \text{otherwise} \end{cases}$

- When the matrix is **symmetric positive semi-definite**:

$$\mathbf{S} = \mathbf{U}\,\Lambda\,\mathbf{U}^T \quad \text{with} \quad \Lambda = \text{diag}\{\lambda_1, \ldots, \lambda_D\}$$

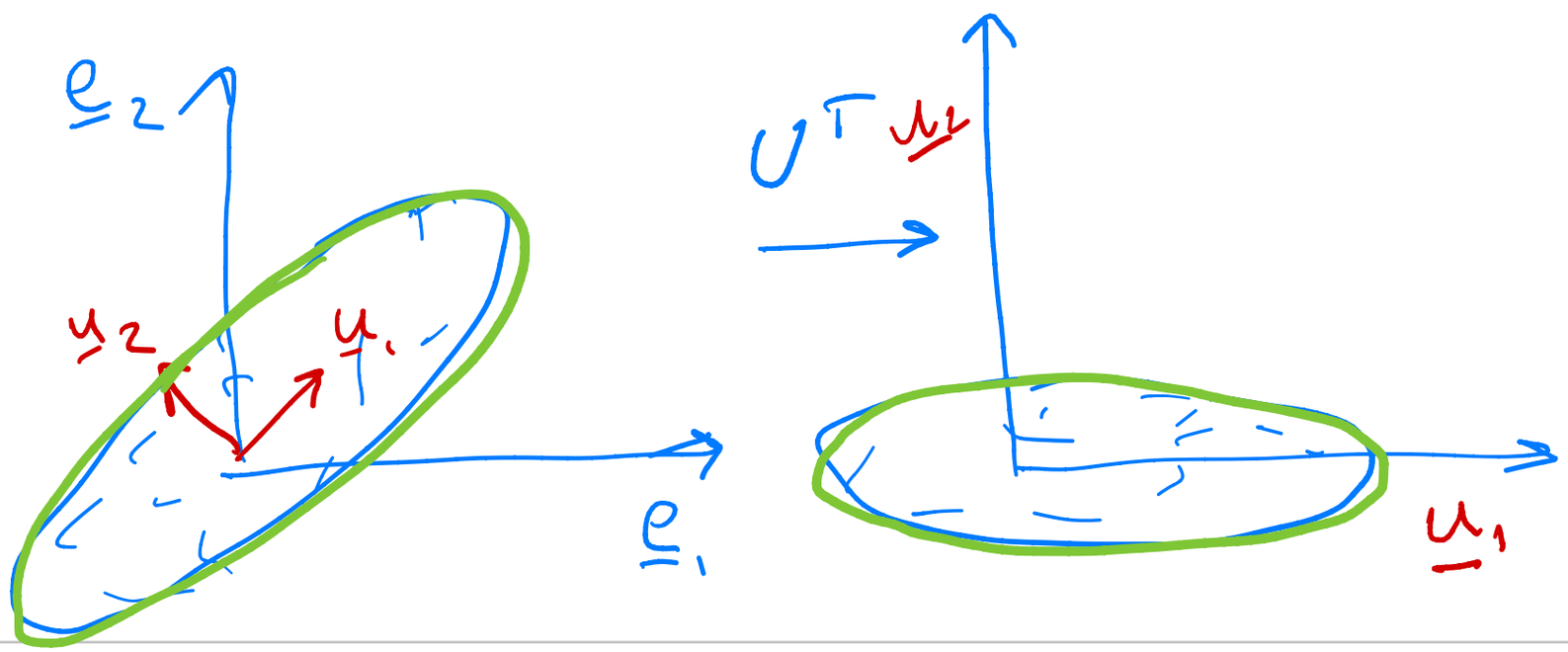
- The eigenvectors are **orthonormal** and are stored in $\mathbf{U} = [\mathbf{u}_1, \ldots, \mathbf{u}_D]$

Change of basis → rotation

- All eigenvalues are **non-negative** and are the elements of the diagonal matrix Λ

$= \text{Tr}(\Lambda U^T U) = \text{Tr}(\Lambda I)$

- Total variance given by $\text{Tr}(\mathbf{S}) = \text{Tr}(\mathbf{U}\,\mathbf{\Lambda}\,\mathbf{U}^T) = \text{Tr}(\mathbf{\Lambda}) = \sum_{i=1}^{D} \lambda_i$



Getting the eigenvectors in practice

- Full eigenvalue decomposition is expensive: $O(D^3)$
- Only need up to the M^{th} component: $O(MD^2)$
- In python:

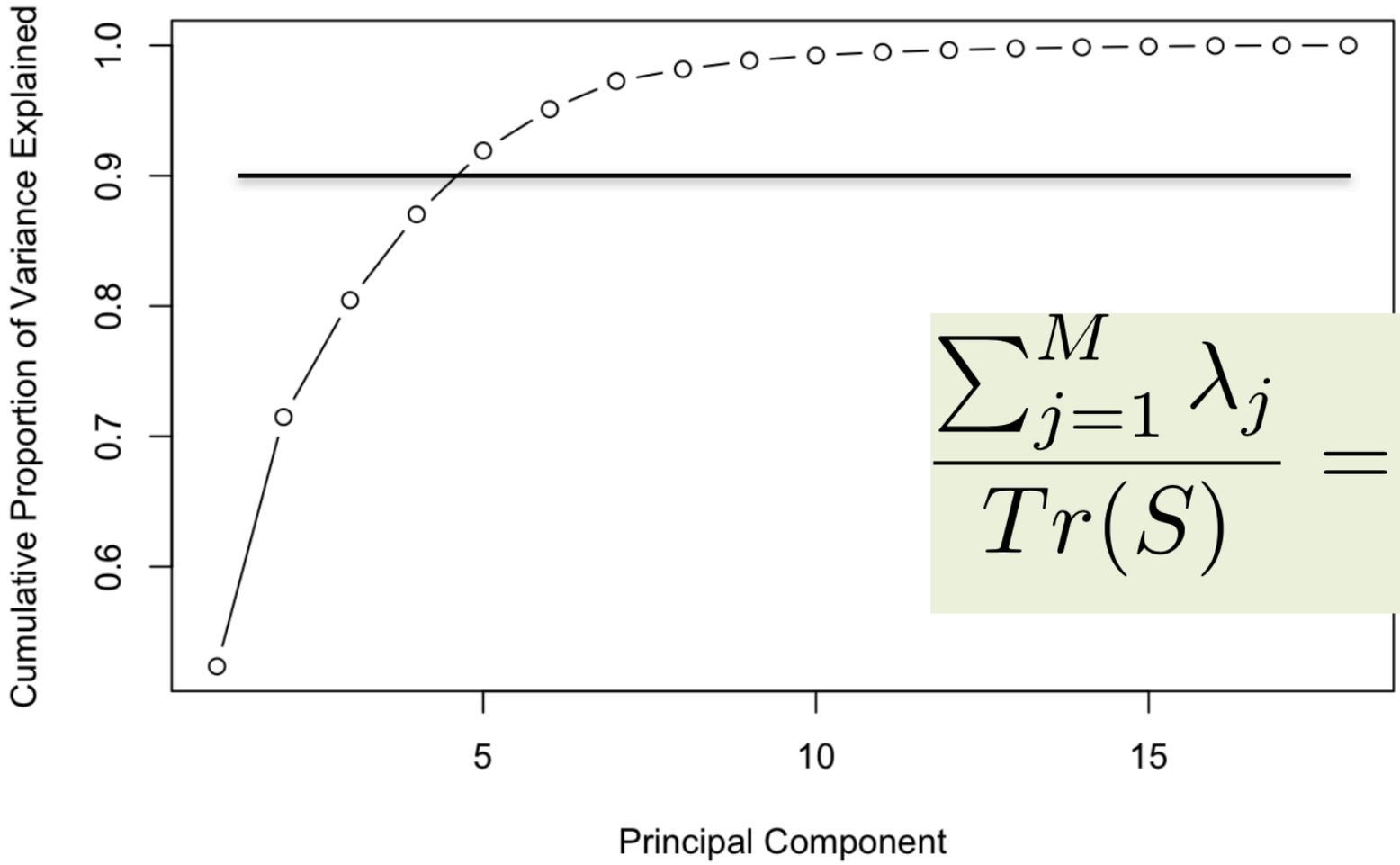
```
M = 10
S = np.cov(X)
Um, Lm, Vm = scipy.sparse.linalg.svds(S, k=M)
```

For symmetric positive definite matrices such as $\mathbf{S}$*, the SVD decomposition is equivalent to the eigen-decomposition*

How to choose M?

- We can measure the discarded variance

- For example to preserve 90% of the variance, pick M such that



The proportion of explained variance

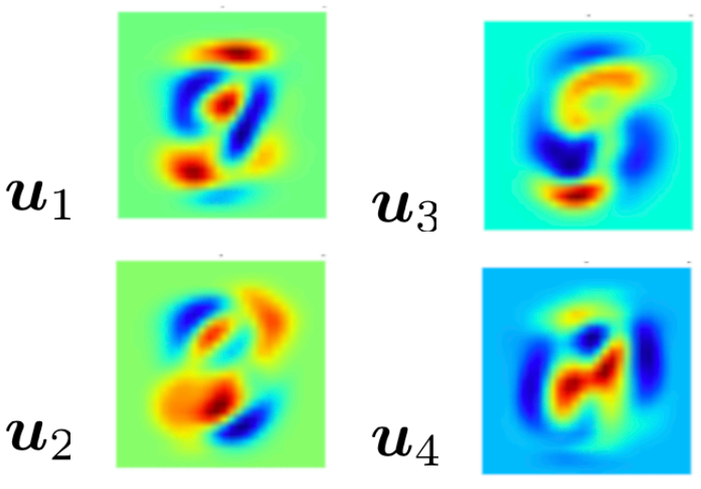
$$\frac{\sum_{j=1}^{M} \lambda_j}{Tr(S)} = \frac{\sum_{j=1}^{M} \lambda_j}{\sum_{j=1}^{D} \lambda_i} > 0.9$$

Applications: dimensionality reduction

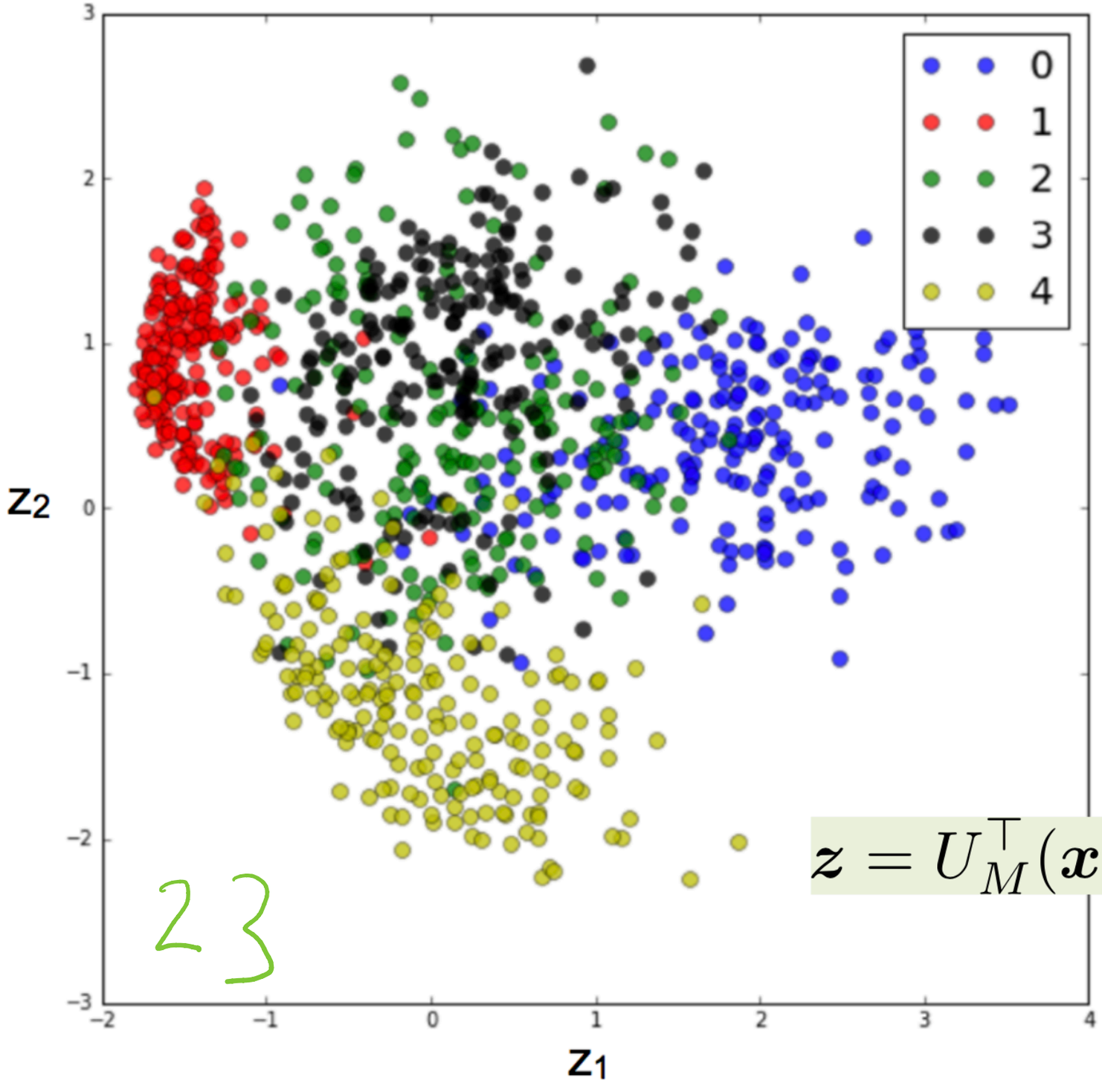
- When data is defined in high dimension (large D) we want to project down to lower dimension because:
  - Reduce time and storage space required
  - For classification/regression: our model **will have less parameters**, thus we need less data points for learning
- Other methods (not covered): **feature selection**. PCA is known as a **feature extraction** method instead.

Applications: 2D Visualization (MNIST)

MNIST: 24 x 24 pixels



Eigenvectors



$$z = U_M^\top (x - \overline{x})$$

Feature Decorrelation

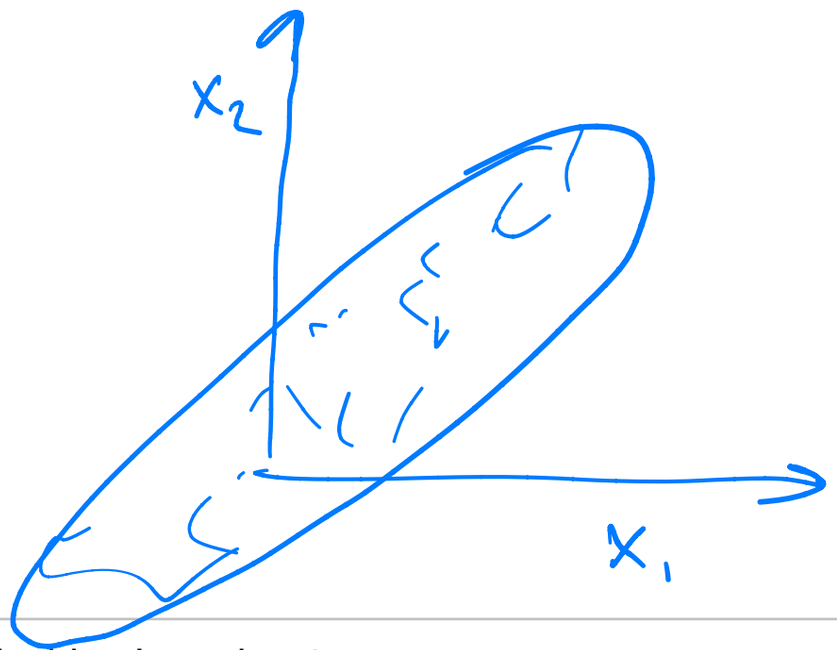
- Good side effect of PCA: features have **no correlation** in the projected space.

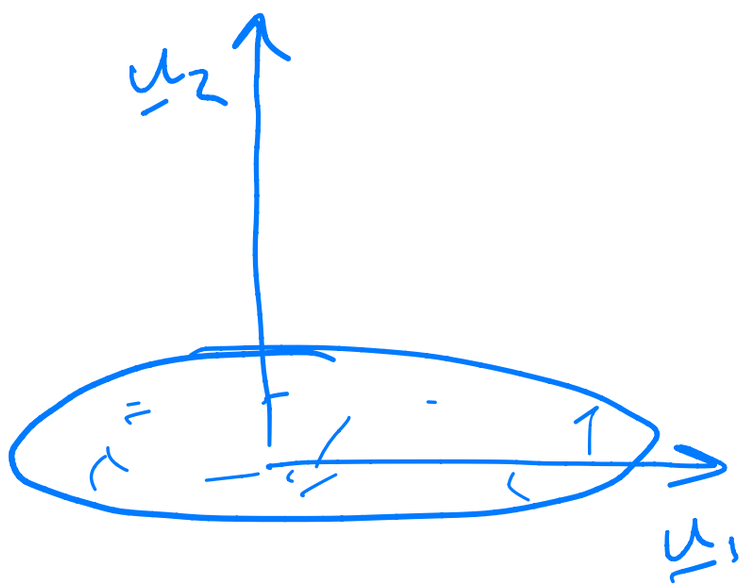
- The covariance matrix of the projected data is **diagonal**

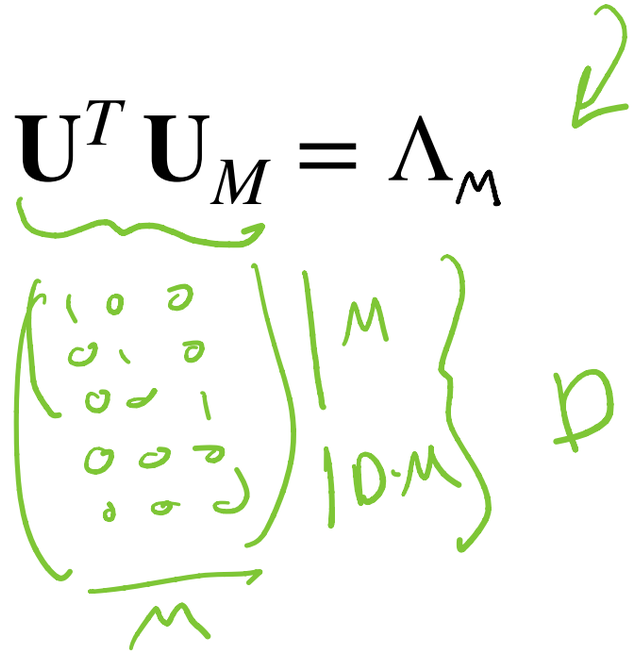
$$\frac{1}{N}\sum_{n=1}^{N}\mathbf{z}_n\mathbf{z}_n^T = \frac{1}{N}\sum_{n=1}^{N}\mathbf{U}_M^T(\mathbf{x}_n-\bar{\mathbf{x}})(\mathbf{x}_n-\bar{\mathbf{x}})^T\mathbf{U}_M$$

$u_i^T S u_i = \lambda_i$

$$= \mathbf{U}_M^T\mathbf{S}\,\mathbf{U}_M = \mathbf{U}_M^T\mathbf{U}\,\mathbf{\Lambda}\,\mathbf{U}^T\mathbf{U}_M = \Lambda_M$$







Applications: whitening (or sphering)

- Before applying learning algorithms we usually do some pre-processing:
  - e.g. **standardization**: subtract the mean and divide by the standard deviation

- With PCA we can **whiten** the data, one step more:
  - **Centre** and **de-correlate** the features:

$$\mathbf{z} = \mathbf{U}_M^T(\mathbf{x} - \bar{\mathbf{x}})$$

  - Cast features to **unit standard deviation** by rescaling:

$$\mathbf{z} = \Lambda_M^{-1/2}\mathbf{U}_M^T(\mathbf{x} - \bar{\mathbf{x}})$$